

=> FILE REG

FILE 'REGISTRY' ENTERED AT 15:45:13 ON 17 JUL 2007

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=> D HIS

FILE 'LREGISTRY' ENTERED AT 15:36:59 ON 17 JUL 2007

L1 STR

FILE 'REGISTRY' ENTERED AT 15:40:32 ON 17 JUL 2007

L2 2 S L1

L3 19 S L1 FUL

SAV L3 BER482/A

FILE 'CAOLD' ENTERED AT 15:44:53 ON 17 JUL 2007

L4 2 S L3

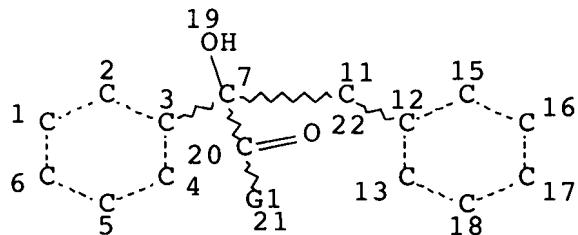
FILE 'ZCA' ENTERED AT 15:45:01 ON 17 JUL 2007

L5 16 S L3

FILE 'REGISTRY' ENTERED AT 15:45:13 ON 17 JUL 2007

=> D L3 QUE STAT

L1 STR



VAR G1=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L3 19 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 598 ITERATIONS

19 ANSWERS

SEARCH TIME: 00.00.01

=> FILE CAOLD

FILE 'CAOLD' ENTERED AT 15:45:23 ON 17 JUL 2007

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

=> D L4 1-2 ALL HITSTR

L4 ANSWER 1 OF 2 CAOLD COPYRIGHT 2007 ACS on STN

AN CA62:15760e CAOLD

TI studies on the electrolytic redn. of ketones - (III) electrolytic  
redn. of aliphatic ketones-studies on cyclohexanone, (IV)  
electrolytic redn. of unsatd. ketones-isophorone, (V) electrolytic  
redn. of aryl alkyl diketones-studies on acetylbenzoyl, (VI)  
electrolytic redn. of aromatic ketones-studies on fluorenone,  
 $\alpha$ -tetralone, acetophenone, and benzophenone

AU Arai, Toshio

IT 78-59-1 529-34-0 579-07-7 1636-34-6 1689-64-1

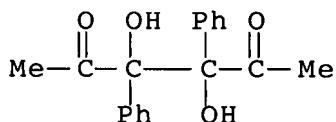
2888-11-1 3073-51-6 3073-53-8 3264-17-3

**3427-06-3**

IT **3427-06-3**

RN 3427-06-3 CAOLD

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA  
INDEX NAME)



L4 ANSWER 2 OF 2 CAOLD COPYRIGHT 2007 ACS on STN  
AN CA59:11299e CAOLD

TI analgesics-abs. configuration of  $\alpha$ -(+)-4-dimethylamino-1,2-diphenyl-3-methyl-2-propionoxybutane, d-propoxyphene

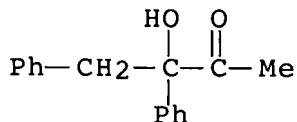
AU Sullivan, Hugh R.; Beck, J. R.; Pohland, A.

IT 2214-31-5 3347-56-6 3536-29-6 5400-92-0 5725-99-5  
5814-85-7 7001-80-1 23271-62-7 35030-49-0 54541-47-8  
**69262-53-9** 83026-52-2 92553-77-0 92903-33-8  
94756-79-3 97080-04-1

IT **69262-53-9**

RN 69262-53-9 CAOLD

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



=> FILE ZCA

FILE 'ZCA' ENTERED AT 15:45:36 ON 17 JUL 2007

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=> D L5 1-16 CBIB ABS HITSTR HITRN

L5 ANSWER 1 OF 16 ZCA COPYRIGHT 2007 ACS on STN

140:391638 Improvement in the storage stability of photoinitiators.

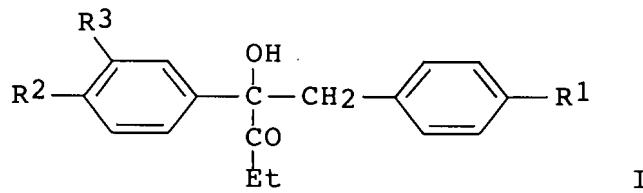
Ulrich, Thomas; Bolle, Thomas; Dietliker, Kurt; Wolf, Jean-Pierre;

Fuchs, Andre (Ciba Specialty Chemicals Holding Inc., Switz.). PCT

Int. Appl. WO 2004037799 A1 20040506, 49 pp. DESIGNATED STATES: W:  
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO,  
CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM,  
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,  
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL,  
PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA,  
UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH,  
CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR,

NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2.  
APPLICATION: WO 2003-EP50729 20031017. PRIORITY: CH 2002-1800  
20021028.

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I

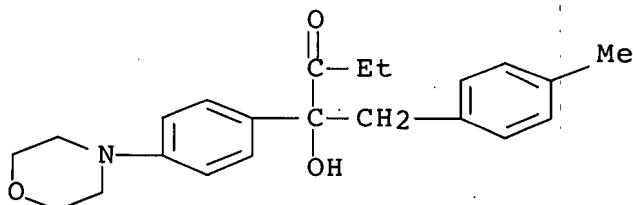
AB Compds. of formula (I), wherein R1 is hydrogen or alkyl; R2 is C1-C4 alkoxy or a morpholino radical; and R3 is hydrogen or C1-C4 alkoxy, are suitable for improving the solv. of specific photoinitiators in formulations and accordingly enhance the storage stability of formulations comprising a photoinitiator and compds. of formula I. Thus, I (R1 = Me, R2 = morpholino, R3 = H) was prepd. from trimethylsilyl cyanide, 4-morpholinobenzaldehyde, Et magnesium bromide, and 4-methylbenzyl bromide.

IT 685523-24-4P

(prepn. of storage stability improvers for photoinitiators)

RN 685523-24-4 ZCA

CN 3-Pentanone, 2-hydroxy-1-(4-methylphenyl)-2-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)

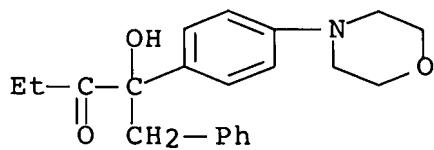


IT 685523-25-5 685523-26-6

(prepn. of storage stability improvers for photoinitiators)

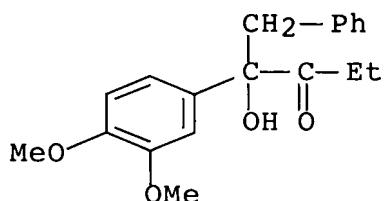
RN 685523-25-5 ZCA

CN 3-Pentanone, 2-hydroxy-2-[4-(4-morpholinyl)phenyl]-1-phenyl- (9CI)  
(CA INDEX NAME)



RN 685523-26-6 ZCA

CN 3-Pantanone, 2-(3,4-dimethoxyphenyl)-2-hydroxy-1-phenyl- (9CI) (CA INDEX NAME)



IT 685523-24-4P

(prepn. of storage stability improvers for photoinitiators)

IT 685523-25-5 685523-26-6

(prepn. of storage stability improvers for photoinitiators)

L5 ANSWER 2 OF 16 ZCA COPYRIGHT 2007 ACS on STN

136:310039 Photochemical reduction of 1,2-diketones in the presence of

TiO<sub>2</sub>. Park, Joon Woo; Hong, Mi Jeung; Park, Kwanghee Koh

(Department of Chemistry, Ewha Womans University, Seoul, 120-750, S.

Korea). Bulletin of the Korean Chemical Society, 22(11), 1213-1216

(English) 2001. CODEN: BKCSDE. ISSN: 0253-2964. OTHER SOURCES:

CASREACT 136:310039. Publisher: Korean Chemical Society.

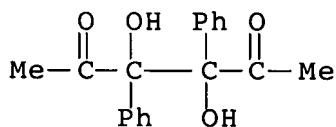
AB 1,2-Diketones, camphorquinone and 1-phenyl-1,2-propanedione, are converted to the corresponding  $\alpha$ -hydroxy ketones in moderate to good yields by TiO<sub>2</sub>-catalyzed photochem. reactions in deoxygenated alc. media. The redn. yield for 1-phenyl-1,2- propanedione is considerably increased by addn. of water or triethylamine.

IT 3427-06-3P

(photochem. redn. of camphorquinone and 1-phenyl-1,2-propanedione in the presence of TiO<sub>2</sub>)

RN 3427-06-3 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 3427-06-3P

(photochem. redn. of camphorquinone and 1-phenyl-1,2-propanedione in the presence of TiO<sub>2</sub>)

L5 ANSWER 3 OF 16 ZCA COPYRIGHT 2007 ACS on STN

## 136:309820 Condensation of stereoisomeric 2-acetyl-2,3-diphenyloxiranes

with ethyl trifluoroacetate. Tyvorskii, V. I.; Pukin, A. V.;

Bobrov, D. N. (Belorussian State University, Minsk, Belarus).

# Chemistry of Heterocyclic Compounds (New York, NY, United States)

1. Khimicheskie Soedineniya (New York, NY, United States) (Translation of Khimiva Geterotsiklichesikh Soedinenij).

37(5), 540-545 (English) 2001. CODEN: CHCCAL. ISSN: 0009-3122

OTHER SOURCES: CASREACT 136:309820. Publisher: Kluwer.

#### OTHER SOURCES: CISREP

**AB** The reaction of *rel*-1-[(2*R*,3*S*)-1,2-Diphenyl-1-oxiranyl]ethanone with Et trifluoroacetate in the presence of sodium isopropoxide gave 3-hydroxy-2,3-diphenyl-6-trifluoromethyl-2,3-dihydro-4*H*-pyran-4-one. Under the same conditions *rel*-1-[(2*R*,3*R*)-1,2-Diphenyl-1-oxiranyl]ethanone forms 2-phenyl-5-(trifluoromethyl)-3-furanol as a result of retro-aldol cleavage of the initial cyclocondensation product.

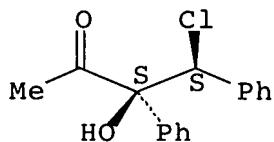
IT 411235-04-6P

(prepn. of 3-furanol derivs. by retro-aldol reaction of Et trifluoroacetate with rel-1-[(2R,3R)-1,2-diphenyl-1-oxiranyl]ethanone)

RN 411235-04-6 ZCA

CN 2-Butanone, 4-chloro-3-hydroxy-3,4-diphenyl-, (3R,4R)-rel- (9CI)  
(CA INDEX NAME)

## Relative stereochemistry.



IT 411235-04-6P

(prepn. of 3-furanol derivs. by retro-aldol reaction of Et trifluoroacetate with rel-1-[*(2R,3R)*-1,2-diphenyl-1-

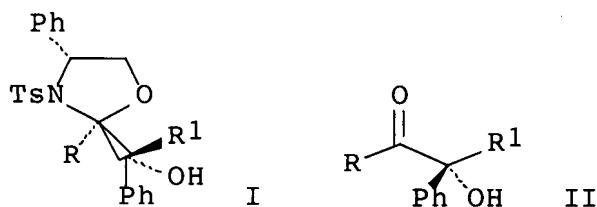
oxiranyl]ethanone)

L5 ANSWER 4 OF 16 ZCA COPYRIGHT 2007 ACS on STN

122:314143 Enantioselective synthesis of  $\alpha$ -branched

$\alpha$ -hydroxy ketones via chiral N-sulfonyl-2-alkyl-2-cyano-1,3-oxazolidines. Harder, Timm; Loehl, Thorsten; Bolte, Michael; Wagner, Kerstin; Hoppe, Dieter (Organisch-Chemisches Inst., Univ. Muenster, Muenster, D-48149, Germany). Tetrahedron Letters, 35(40), 7365-8 (English) 1994. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 122:314143.

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AB The stereochem. homogeneous title oxazolidines, prep'd. in two steps from orthoesters and N-tosylphenylglycinol, afford with two sequential Grignard addns. predominantly the tertiary alcs. I (R = Me, Et; R1 = Me, PhCH2, allyl). Electrochem. detosylation, followed by aq. work up, yields enantiomerically enriched ketones II.

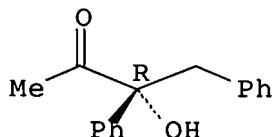
IT 161977-52-2P 161977-53-3P

(enantioselective synthesis of hydroxy ketones via chiral sulfonylalkylcyanooxazolidines)

RN 161977-52-2 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl-, (R)- (9CI) (CA INDEX NAME)

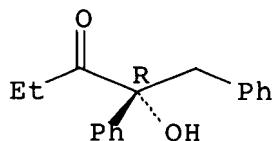
Absolute stereochemistry.



RN 161977-53-3 ZCA

CN 3-Pentanone, 2-hydroxy-1,2-diphenyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 161977-52-2P 161977-53-3P

(enantioselective synthesis of hydroxy ketones via chiral  
sulfonylalkylcyanooxazolidines)

L5 ANSWER 5 OF 16 ZCA COPYRIGHT 2007 ACS on STN

122:313938 The effects of counterion and solvent on the reactivity of nickel acylate complexes. La Duca, Melissa J. T.; Simunic, Joan L.; Hershberger, James W.; Pinhas, Allan R. (Department of Chemistry, University of Cincinnati, Cincinnati, OH, 45221-0172, USA).

Inorganica Chimica Acta, 222(1-2), 165-77 (English) 1994. CODEN: ICHAA3. ISSN: 0020-1693.

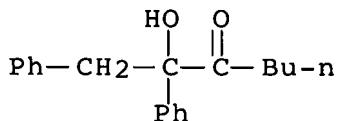
AB Nickel acylate complexes, which can be generated starting with a carbon, nitrogen or oxygen nucleophile, act as acyl anion equiv. and therefore are an excellent method of assembling complex org. mols. from readily available starting materials. In an effort to increase the synthetic utility of these easily formed reagents, a systematic study of the reactivity of the nickel acylate complex generated under a variety of conditions was performed. Those acylate complexes generated with a carbon based nucleophile, such as a Bu or Ph anion, show a large change in reactivity upon changing, for example, the solvent from THF to Et<sub>2</sub>O or the counterion from Li<sup>+</sup> to MgCl<sup>+</sup>. This reactivity change is due to a large change in the structure of the acylate complex with a different counterion or solvent, as detd. by IR and <sup>13</sup>C NMR spectroscopy and by oxidn. potentials. In contrast, when a heteroatom nucleophile is used, such as a dialkyl amide or an alkoxide, the effect of a change in solvent or counterion on the structure, and therefore on the reactivity of the acylate complex, is minimal.

IT 163337-45-9P

(effects of counterion and solvent on the reactivity of nickel acylate complexes)

RN 163337-45-9 ZCA

CN 3-Heptanone, 2-hydroxy-1,2-diphenyl- (9CI) (CA INDEX NAME)



IT 163337-45-9P

(effects of counterion and solvent on the reactivity of nickel acylate complexes)

L5 ANSWER 6 OF 16 ZCA COPYRIGHT 2007 ACS on STN

114:5915 Regioreversed allylation in Lewis acid-mediated and

photochemical addition reactions of unsymmetric  $\alpha$ -diketones with allylic stannanes. Takuwa, Akio; Nishigaichi, Yutaka;

Yamashita, Koichi; Iwamoto, Hidetoshi (Fac. Sci., Shimane Univ., Matsue, 690, Japan). Chemistry Letters (9), 1761-4 (English) 1990.

CODEN: CMLTAG. ISSN: 0366-7022. OTHER SOURCES: CASREACT 114:5915.

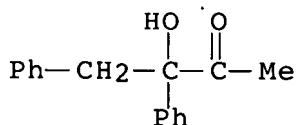
AB In the photochem. reaction of allyl- and benzyltrimethylstannane with unsym.  $\alpha$ -diketones PhCOCOR, the allylic group was introduced to the benzoyl carbon in high or excellent selectivity, whereas the acyl carbon was allylated either exclusively or predominantly under  $\text{BF}_3$ -mediated reaction.

IT 69262-53-9P 130925-75-6P

(prepn. of)

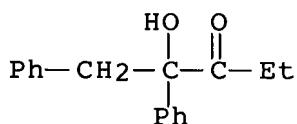
RN 69262-53-9 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



RN 130925-75-6 ZCA

CN 3-Pentanone, 2-hydroxy-1,2-diphenyl- (9CI) (CA INDEX NAME)



IT 69262-53-9P 130925-75-6P

(prepn. of)

L5 ANSWER 7 OF 16 ZCA COPYRIGHT 2007 ACS on STN

111:96764 Radical addition to carbonyl carbon promoted by aqueous

titanium trichloride: stereoselective synthesis of

$\alpha,\beta$ -dihydroxy ketones. Clerici, Angelo; Porta, Ombretta

(Dip. Chim., Politec. Milano, Milan, 20133, Italy). Journal of

Organic Chemistry, 54(16), 3872-8 (English) 1989. CODEN: JOCEAH.  
ISSN: 0022-3263. OTHER SOURCES: CASREACT 111:96764.

AB Ketyl radicals, formed by chemoselective Ti(III) redn. of  $\alpha,\beta$ -dicarbonyl compds., add to the carbonyl carbon of aldehydes under mild conditions to afford  $\alpha,\beta$ -dihydroxy ketones in good to excellent yields. Simple diastereoselectivity strongly depends on the bulk of groups bonded to both the ketyl radical and the aldehydic function. The relative configuration of two of the keto diols was established by single-crystal x-ray diffractometry.

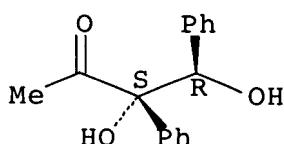
IT 122171-90-8P

(prepn. of)

RN 122171-90-8 ZCA

CN 2-Butanone, 3,4-dihydroxy-3,4-diphenyl-, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 122171-90-8P

(prepn. of)

L5 ANSWER 8 OF 16 ZCA COPYRIGHT 2007 ACS on STN

102:131639 Facile preparation of 3-aryl-2-hydroxy-1-propanones by the Grignard-type addition of benzyl halides to 1,2-diketones mediated by metallic nickel. Inaba, Shinichi; Rieke, Reuben D. (Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA). Synthesis (10), 844-5 (English) 1984. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 102:131639.

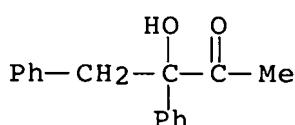
AB RCH<sub>2</sub>CR<sub>1</sub>(OH)COR<sub>2</sub> (R = Ph, 4-MeC<sub>6</sub>H<sub>4</sub>, 3-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>, 4-FC<sub>6</sub>H<sub>4</sub>, 4-CIC<sub>6</sub>H<sub>4</sub>, 4-BrC<sub>6</sub>H<sub>4</sub>, 4-NCC<sub>6</sub>H<sub>4</sub>, 4-MeO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>, 1-naphthyl; R<sub>1</sub>, R<sub>2</sub> = Ph, Me) were obtained in 35-83% yield by treating RCH<sub>2</sub>R<sub>3</sub> (R<sub>3</sub> = Cl, Br) with R<sub>1</sub>COCOR<sub>2</sub> in the presence of Ni.

IT 69262-53-9P

(prepn. of)

RN 69262-53-9 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



IT 69262-53-9P  
(prepn. of)

L5 ANSWER 9 OF 16 ZCA COPYRIGHT 2007 ACS on STN  
99:157554 Base catalyzed rearrangements involving ylide intermediates.

Part 18. Competing [1,2], [1,3], and [1,4] rearrangements of ammonium ylides. Chantrapromma, Kan; Ollis, W. David; Sutherland, Ian O. (Dep. Chem., Univ. Sheffield, Sheffield, S3 7HF, UK).

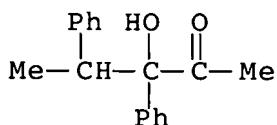
Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (5), 1049-61 (English) 1983.

CODEN: JCPRB4. ISSN: 0300-922X. OTHER SOURCES: CASREACT 99:157554.

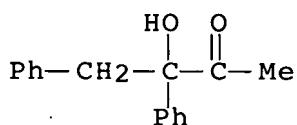
AB The mechanisms of the competing [1,2]-, [1,3]-, and [1,4]-rearrangements of benzyl- and phenylethylammonium ylides were studied. E.g., rearrangement of PhCOC-MeN+Me<sub>2</sub>CH<sub>2</sub>Ph were largely intramol., with the intermolecularity of the [1,2]- and [1,3]-rearrangements being <28% and of the [1,4]-rearrangements being 14% in MeOH at 55°. Competing [1,2]- and [1,3]-rearrangements of optically active benzylammonium ylides, e.g. PhCOC-MeN+MeCHMePh, occurred with predominantly retention of configuration of the migrating group, but the intramol. stereoselectivity of the [1,2]-rearrangement was much greater than that of the [1,3]-rearrangement. The mechanism involves a radical pair path for all 3 rearrangements.

IT 69262-63-1P  
(prepn. and degrdn. of)

RN 69262-63-1 ZCA  
CN 2-Pentanone, 3-hydroxy-3,4-diphenyl- (9CI) (CA INDEX NAME)



IT 69262-53-9P  
(prepn. and redn. of)  
RN 69262-53-9 ZCA  
CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



IT 69262-60-8P 69303-25-9P 87258-78-4P

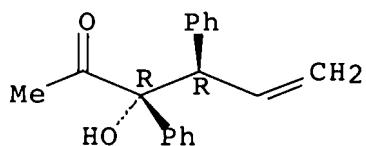
87258-79-5P

(prepn. of, by base-catalyzed rearrangement of acylammonium ylide)

RN 69262-60-8 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R\*,R\*)- (9CI) (CA INDEX NAME)

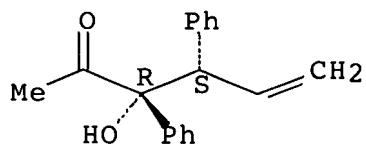
Relative stereochemistry.



RN 69303-25-9 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R\*,S\*)- (9CI) (CA INDEX NAME)

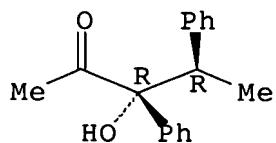
Relative stereochemistry.



RN 87258-78-4 ZCA

CN 2-Pentanone, 3-hydroxy-3,4-diphenyl-, (R\*,R\*)- (9CI) (CA INDEX NAME)

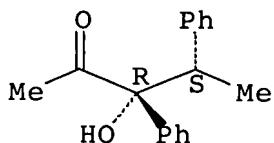
Relative stereochemistry.



RN 87258-79-5 ZCA

CN 2-Pentanone, 3-hydroxy-3,4-diphenyl-, (R\*,S\*)- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.



IT 69262-63-1P

(prepn. and degrdn. of)

IT 69262-53-9P

(prepn. and redn. of)

IT 69262-60-8P 69303-25-9P 87258-78-4P

87258-79-5P

(prepn. of, by base-catalyzed rearrangement of acylammonium ylide)

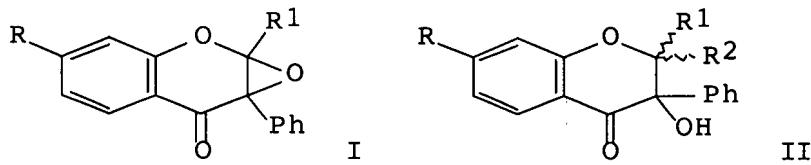
L5 ANSWER 10 OF 16 ZCA COPYRIGHT 2007 ACS on STN

94:30492 Studies in the chemistry of chromone epoxides. Donnelly, John

A.; Keegan, John R.; Quigley, Killian (Chem. Dep., Univ. Coll., Dublin, Ire.). Tetrahedron, 36(11), 1671-80 (English) 1980. CODEN:

TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 94:30492.

GI



AB Chromones and isoflavones were epoxidized by alk. H<sub>2</sub>O<sub>2</sub> and their reactions studied. E.g., epoxide I (R = MeO, R1 = H) underwent regioselective acid-catalyzed ring cleavage to 3-hydroxychromanone II (R = MeO, R1 =  $\alpha$ -OEt, R2 =  $\beta$ -H), whereas acidic hydrolysis gave a 1,2-diol II (R = MeO, R1 = OH, R2 = H). A similar compd. was obtained by cyclizing 2-BzOC<sub>6</sub>H<sub>4</sub>COCHBr<sub>2</sub>. In contrast, epoxide I (R = H, R1 = Me) with BF<sub>3</sub>·OEt<sub>2</sub> gave fluorohydrin II (R = H, R1 = Me, R2 = F) and acid- and base-

catalyzed hydrolysis gave a 1,3- and a 1,2-diketone, resp. This epoxide formed a cyclic sulfate with H<sub>2</sub>SO<sub>4</sub>.

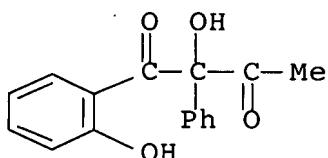
IT 76182-84-8P

(prepn. of)

RN 76182-84-8 ZCA

CN 1,3-Butanedione, 2-hydroxy-1-(2-hydroxyphenyl)-2-phenyl- (9CI) (CA

INDEX NAME)



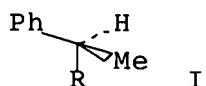
IT 76182-84-8P

(prepn. of)

L5 ANSWER 11 OF 16 ZCA COPYRIGHT 2007 ACS on STN

90:86594 Stereoselectivities in competing [1,2] and [1,3] rearrangements. Chantrapromma, Kan; Ollis, W. David; Sutherland, Ian O. (Dep. Chem., Univ. Sheffield, Sheffield, UK). Journal of the Chemical Society, Chemical Communications (15), 672-3 (English) 1978. CODEN: JCCCAT. ISSN: 0022-4936.

GI



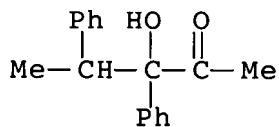
AB The competing intramol. [1,2] and [1,3] rearrangements of chiral ylide I (R = PhCOC-MeN+Me<sub>2</sub>), generated by treatment of I (R = PhCOCHMeN+Me<sub>2</sub>BF<sub>4</sub>-) with base, to give I [R = PhCOCMe(NMe<sub>2</sub>), MeCOC(OH)Ph, resp.] are both stereoselective and occur with predominant retention of configuration of the migrating phenylethyl group. The stereoselectivity of the [1,2] rearrangement exceeds significantly that of the [1,3] rearrangement. The unusually high stereoselectivity of the [1,2] Stevens rearrangement is a consequence of the limited translational motion required within the radical pair before intramol. [1,2] coupling can occur.

IT 69262-63-1P

(prepn. and abs. configuration of)

RN 69262-63-1 ZCA

CN 2-Pentanone, 3-hydroxy-3,4-diphenyl- (9CI) (CA INDEX NAME)



IT 69262-63-1P

(prepn. and abs. configuration of)

L5 ANSWER 12 OF 16 ZCA COPYRIGHT 2007 ACS on STN

90:86448 Radical coupling products derived from ammonium ylides.

Competing [1,2], [1,3], and [1,4] anionic rearrangements.

Chantrapromma, Kan; Ollis, W. David; Sutherland, Ian O. (Dep. Chem., Univ. Sheffield, Sheffield, UK). Journal of the Chemical Society, Chemical Communications (15), 670-1 (English) 1978. CODEN: JCCCAT.

ISSN: 0022-4936.

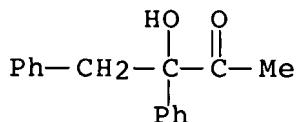
AB Thermal rearrangement of PhCOC-MeN+Me2CH2Ph (I), generated by treating PhCOCHMeN+Me2CH2Ph Br- with aq. NaOH, gave 86% PhCOCMe(CH2Ph)NMe2, 6% HOCMePhCOCH2Ph and 2% MeOCHPhCOCH2Ph by [1,2], [1,3] and [1,4] paths, resp. The intramolecularity of these processes was studied and showed that the rearrangement occurs via a radical-pair mechanism involving initial homolysis of I, followed by 3 possible modes of radical-pair recombination. For allylammonium ylides the no. of possible coupling modes is further increased.

IT 69262-53-9P 69262-60-8P 69303-25-9P

(prepn. of)

RN 69262-53-9 ZCA

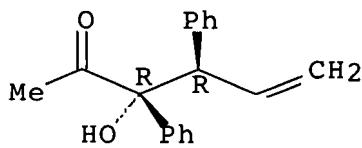
CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



RN 69262-60-8 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R\*,R\*)- (9CI) (CA INDEX NAME)

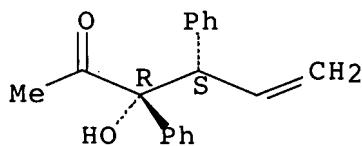
Relative stereochemistry.



RN 69303-25-9 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 69262-53-9P 69262-60-8P 69303-25-9P

(prepn. of)

L5 ANSWER 13 OF 16 ZCA COPYRIGHT 2007 ACS on STN

87:52424 Photochemistry of some cyclopropyl conjugated 1,2-diketones.

Part 2. Fragmentation reactions and reduction by aldehydes.

Kelder, J.; Cefontain, H.; Van der Wielen, F. W. M. (Lab. Org.

Chem., Univ. Amsterdam, Amsterdam, Neth.). Journal of the Chemical

Society, Perkin Transactions 2: Physical Organic Chemistry

(1972-1999) (5), 710-14 (English) 1977. CODEN: JCPKBH. ISSN:

0300-9580.

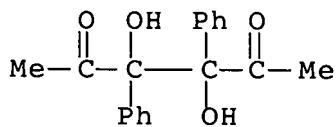
AB The photochem. of 3 cyclopropyl conjugated and some related 1,2-diketones in C<sub>6</sub>H<sub>6</sub> in the absence and presence of MeCHO or formylcyclopropane as H donor was studied. In C<sub>6</sub>H<sub>6</sub> no photodecompn. occurred at  $\lambda > 403$  nm, but at  $> 300$  nm and  $< 403$  nm the 1,2-diketones, with the exception of dicyclopropylethanedione (I), decompd. The products arise from initial bond rupture between the carbonyl groups, subsequent decarbonylation of part of the acyl radicals, and recombination. On irradn. of a I-biacetyl mixt., acyl interchange was obsd. The photoreaction of the 1,2-diketones in the presence of aliph. aldehyde gave dihydrodimers,  $\alpha,\alpha$ - diacylalkanols, and esters.

IT 3427-06-3P

(prepn. of)

RN 3427-06-3 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 3427-06-3P  
(prepn. of)

L5 ANSWER 14 OF 16 ZCA COPYRIGHT 2007 ACS on STN  
82:42630 Photochemical reactions of some 1-aryl-1,2-propanediones.

Ogata, Yoshiro; Takagi, Katsuhiko (Fac. Eng., Nagoya Univ., Nagoya, Japan). Bulletin of the Chemical Society of Japan, 49(7), 2255-9 (English) 1974. CODEN: BCSJA8. ISSN: 0009-2673.

GI For diagram(s), see printed CA Issue.

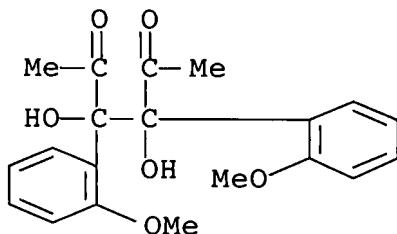
AB Irradn. of 1-aryl-1,2-propanediones (I; R = H, p-OMe, o-OMe, O-Me) in 2-propanol gives pinacols or hydrols formed by redn. at the aroyl (but not acetyl) O. The products from I (R = o-Me) can also be accounted for by initial H abstraction from ortho Me by the aroyl carbonyl O. Their photoreactivities are discussed in relation to their electronic emission spectra and triplet configuration.

IT 53583-02-1P

(prepn. of)

RN 53583-02-1 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-bis(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT 53583-02-1P  
(prepn. of)

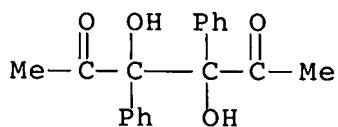
L5 ANSWER 15 OF 16 ZCA COPYRIGHT 2007 ACS on STN  
62:88544 Original Reference No. 62:15760g-h Studies on the electrolytic reduction of ketones. V. The electrolytic reduction of aryl alkyl diketones. Studies on acetylbenzoyl. Arai, Toshio (Shinshu Univ., Nagano, Japan). Denki Kagaku, 30(3), 175-8 (Unavailable) 1962. CODEN: DNKKA2. ISSN: 0366-9440.

AB MeCOCOPh (I) gave 2 half-wave potentials (-0.235 to -0.265, and -0.82 to -0.85 v.) at pH < 3. At pH 3-8, the 1st wave shifted from -0.35 to -0.74 v., and the 2nd wave was not observed. No reductive half-wave was recognized at pH > 10. The remarkably low potential of the 1st wave at pH < 3 was ascribed to the conjugation of C:O with the phenyl group. The 1st wave was concluded to be a 1-electron redn. wave on the basis of formation of  $\alpha,\beta$ - diacetylhydrobenzoin (II), m. 118.5°. Use of Cu or Sn in redn. of 5 g. I in ethanolic 0.2N H<sub>2</sub>SO<sub>4</sub> at 15-8° gave 1.5 or 2.2 g. II. No redn. product was obtained when Cd was used. Redn. of I with a Hg anode gave an organomercuric compd., m. 80° presumably PhCH<sub>2</sub>CHMeHgCl.

IT 3427-06-3P, 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl-  
(formation of, in acetylbenzoyl electrolytic redn.)

RN 3427-06-3 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA  
INDEX NAME)



IT 3427-06-3P, 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl-  
(formation of, in acetylbenzoyl electrolytic redn.)

L5 ANSWER 16 OF 16 ZCA COPYRIGHT 2007 ACS on STN  
59:61744 Original Reference No. 59:11299d-h,11300a-d Analgesics.

Absolute configuration of  $\alpha$ -(+)-4-dimethyl-amino-1,2-diphenyl-3-methyl-2-propionoxybutane, d-propoxyphene. Sullivan, H. R.; Beck, J. R.; Pohland, A. (Eli Lilly & Co., Indianapolis, IN). Journal of Organic Chemistry, 28(9), 2381-5 (Unavailable) 1963. CODEN: JOCEAH.  
ISSN: 0022-3263.

GI For diagram(s), see printed CA Issue.

AB  $\alpha$ -(+)-Me<sub>2</sub>NCH<sub>2</sub>CHMeCPh(CH<sub>2</sub>Ph)O<sub>2</sub>CEt.HCl (I) (15 g.) and 135 mL 5N HCl was refluxed 2 h. and concd. to dryness to give 8.5 g.  $\alpha$ -(+)-Me<sub>2</sub>NCH<sub>2</sub>CHMeCPh:CHPh.HCl (II), m. 189-90° (MeOH-EtOAc),  $[\alpha]$  (all 25/D) -33.7° (c 1, H<sub>2</sub>O). Similarly, 50 g.  $\alpha$ -(+)-isomer of I gave 21 g. II  $\alpha$ -(+)-isomer (III), m. 189-90°,  $[\alpha]$  34.3° (c 1, H<sub>2</sub>O). Into 25 g. II, 150 mL MeOH, and 1100 mL EtOAc at -20° was passed O<sub>3</sub> in excess; the whole added to 250 mL ice-H<sub>2</sub>O, kept overnight, the MeOH and EtOAc distd. in vacuo, the aq. soln. washed with Et<sub>2</sub>O (conc. of these gave BzH), the aq. soln. treated with excess aq. NH<sub>3</sub>, extd. with Et<sub>2</sub>O, and the Et<sub>2</sub>O, exts. dried and treated with dry HCl gave 8 g.  $\alpha$ -(+)-Me<sub>2</sub>NCH<sub>2</sub>CHMeBz.HCl (IV), m. 153-4° (MeOH-EtOAc),  $[\alpha]$  -47° (c 1, H<sub>2</sub>O). To 11.8 g. IV, 130 g. anhyd. Na<sub>2</sub>HPO<sub>4</sub>, and 300 mL CH<sub>2</sub>Cl<sub>2</sub> at 0-5° was added CF<sub>3</sub>-CO<sub>3</sub>H [from 50.8 g. (CF<sub>3</sub>CO)<sub>2</sub>O, 8.2 mL 90% H<sub>2</sub>O<sub>2</sub>, and 100 mL CH<sub>2</sub>Cl<sub>2</sub>, at 0°]; the whole stirred 1 h. (temp. rise to 10°), the solid mixt. kept 4 h. at room temp., 200 mL H<sub>2</sub>O added, the CH<sub>2</sub>Cl<sub>2</sub> phase sepd., evapd. to dryness, the residue dissolved in 100 mL 2N HCl, washed, treated with excess concd. aq. NH<sub>3</sub> and extd. with Et<sub>2</sub>O and the dried Et<sub>2</sub>O soln. treated with dry HCl gave 3.8 g.  $\alpha$ -(+)-Me<sub>2</sub>NCH<sub>2</sub>CHMeOBz.HCl, m. 160-1° (MeOH-

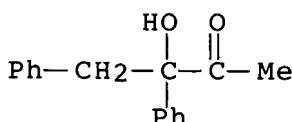
EtOAc),  $[\alpha]$  -62.8° (c 1, H<sub>2</sub>O). D(-)-H<sub>2</sub>NCH<sub>2</sub>CH- (OH)Me.HCl (2.7 g.), 1.6 g. HCO<sub>2</sub>Na, 8.3 g. 100% HCO<sub>2</sub>H, and 6.7 g. 37% HCHO were refluxed 14 h. to give 3.13 g. hygroscopic D(--)-Me<sub>2</sub>NCH<sub>2</sub>CH(OH)Me.HCl (V),  $[\alpha]$  -44.5° (c 1, MeOH); V, 7.1 g. BzCl, 25 mL. Et<sub>3</sub>N, and 80 mL. CHCl<sub>3</sub> refluxed 1 h. gave 4.2 g. Me<sub>2</sub>NCH<sub>2</sub>CH(OBz)Me, HCl, m. 160-1° (MeOH-EtOAc),  $[\alpha]$  -63.3° (c 1, H<sub>2</sub>O). I (370 g.), 4.5 l. MeOH, and 650 mL. 30% H<sub>2</sub>O<sub>2</sub> kept 48 h. at room temp., the whole evapd. to dryness, 0.4 g. PtO<sub>2</sub> added (caution), filtered, the filtrate evapd. to dryness, and the residue in 2 l. EtOAc treated with 40 g. HCl in 1 l. EtOAc gave 370 g. I N-oxide-HCl (VI), m. 186-7° (MeOH EtOAc),  $[\alpha]$  20.2° (c 2, MeOH); VI in 1500 mL. H<sub>2</sub>O satd. with K<sub>2</sub>CO<sub>3</sub> and extd. with Et<sub>2</sub>O gave 320 g. N-oxide (VII); VII heated slowly at 0.5 mm. to 140°, kept 0.5 h. at 140°, the whole cooled, dissolved in Et<sub>2</sub>O and the Et<sub>2</sub>O soln. washed, dried, concd. and distd. gave 200 g. (+)-CH<sub>2</sub>:CMeCPh(CHPh)O<sub>2</sub>CEt (VIII), b0.6 152°, n<sub>25</sub>D 1.5466,  $[\alpha]$  97° (c 1.3, Me<sub>2</sub>CO) (the cold trap from the pyrolysis contained Me<sub>2</sub>NHOH). VIII (45 g.) in 1 l. EtOAc at -50° and O<sub>3</sub> to blue color, the whole poured into ice-H<sub>2</sub>O, kept overnight, dil. aq. NaHSO<sub>3</sub> added, dropwise, to neg. starch-iodide test, the EtOAc soln. sepd., washed and dried gave 41 g. (+)-AcCPh-(O<sub>2</sub>CEt)CH<sub>2</sub>Ph (IX), b0.5 156-7°,  $[\alpha]$  182.7° (c 1.1, Me<sub>2</sub>CO). IX (32.5 g.), 1 l. 5N HCl, and 1 l. EtOH refluxed 20 h. gave 21.9 g. (+)-AcC(OH)PhCH<sub>2</sub>Ph (X), b0.5 148°, n<sub>25</sub>D 1.5660,  $[\alpha]$  141° (c 1.3, EtOH). To 60 g. X in 200 mL. glacial AcOH was added, dropwise, 45 g. Br in 100 mL. glacial AcOH, and the whole stirred 1 h. and evapd. to dryness in vacuo; the residue in 600 mL. C<sub>5</sub>H<sub>5</sub>N heated 1 h. at 100°, the whole concd., and the residue and 60 g. NaOH in 900 mL. H<sub>2</sub>O heated 2 h. at 100° gave 20 g. (-)-PhCH<sub>2</sub>C(OH)PhCO<sub>2</sub>H (XI), m. 145-6° (aq. EtOH),  $[\alpha]$  13.7° (c 3.5, EtOH). XI (18 g.), 40 g. Ag<sub>2</sub>O and 200 mL. MeI refluxed and stirred 3 h. gave 15 g. Me ester (XII), m. 102-3° (Et<sub>2</sub>O-petr. ether),  $[\alpha]$  -32.4° (c 3.4, CHCl<sub>3</sub>). Abs. EtOH, (200 mL.) and 60 g. freshly prep'd. W-2 Raney Ni, shaken first with 40 lb./in.2 H, 8 g. XII added, and the whole refluxed 8 h., filtered, the residue from the concn. of the filtrate dissolved in 40 mL. petr. ether, 1.4 g. XII which sepd., filtered off, the filtrate evapd. and the residue distd. gave 6 g. (+)-PhCH<sub>2</sub>CHPhCO<sub>2</sub>Me (XIII), b0.2 123-4°, n<sub>25</sub>D 1.5518,  $[\alpha]$  -90.5° (c 4.6, CHCl<sub>3</sub>). To 1.7 g. LiAlH<sub>4</sub> in 110 mL. anhyd. Et<sub>2</sub>O was added 10.2 g. XIII in 40 mL. Et<sub>2</sub>O, dropwise, and the whole refluxed 3 h. to give 7.8 g. (+)-PhCH<sub>2</sub>CHPhCH<sub>2</sub>OH, b0.2 128°, n<sub>25</sub>D 1.5742,  $[\alpha]$  76.3°; tosylate (XIV) (prep'd. in C<sub>5</sub>H<sub>5</sub>N), m. 89-90° (Me<sub>2</sub>CO-petr. ether),  $[\alpha]$  40.2° (c 2.4, Me<sub>2</sub>CO). XIV (7.4 g.), 16.5 g. NaI, and 200 mL. anhyd. Me<sub>2</sub>CO refluxed and stirred 20 h. gave 6.35 g. (+)-PhCH<sub>2</sub>CHPhCH<sub>2</sub>I (XV), m. 54-5° (petr. ether),  $[\alpha]$  16.6° (c 3.9, EtOH); XV, 3.0 g. NaHCO<sub>3</sub>, 150 mL. abs. EtOH, and 5 g. Pd-C hydrogenated 10 h. at 25° gave 2.6 g. (+)-PhCH<sub>2</sub>CHPhMe, b0.3 85°, n<sub>25</sub>D 1.5558,  $[\alpha]$  76.7° (c 2.3, CHCl<sub>3</sub>). (-)-threo-PhCH(OH)CHPhMe (1.4 g.) added to 100 mL. abs. EtOH and 30 g. W-2 Raney Ni, shaken first in H as above, and the whole refluxed 8 h. gave 1.15 g. D(-)-PhCH<sub>2</sub>CHPhMe, b0.5 88°, n<sub>25</sub>D 1.5553,  $[\alpha]$  -76.3° (c 2.2, CHCl<sub>3</sub>). The abs. configuration of I is (2S.3R).

IT 69262-53-9P, 2-Butanone, 3-hydroxy-3,4-diphenyl-

(prepn. of)

RN 69262-53-9 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



IT **69262-53-9P**, 2-Butanone, 3-hydroxy-3,4-diphenyl-  
(prepn. of)